wwPDB NMR Structure Validation Summary Report

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PDB ID	:	1BCI
Title	:	C2 DOMAIN OF CYTOSOLIC PHOSPHOLIPASE A2, NMR, MINIMIZED AVERAGE STRUCTURE
Authors	:	Xu, G.Y.; Mcdonagh, T.; Yu, H.A.; Nalefski, E.A.; Clark, J.D.; Cumming, D.A.
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

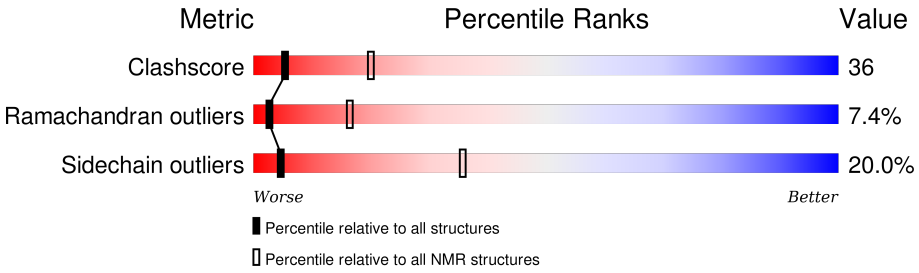
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	138	31% 46% 12% 11%

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1967 atoms, of which 973 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYTOSOLIC PHOSPHOLIPASE A2.

Mol	Chain	Residues	Atoms						Trace
1	A	123	Total	C	H	N	O	S	0
			1965	634	973	157	195	6	

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

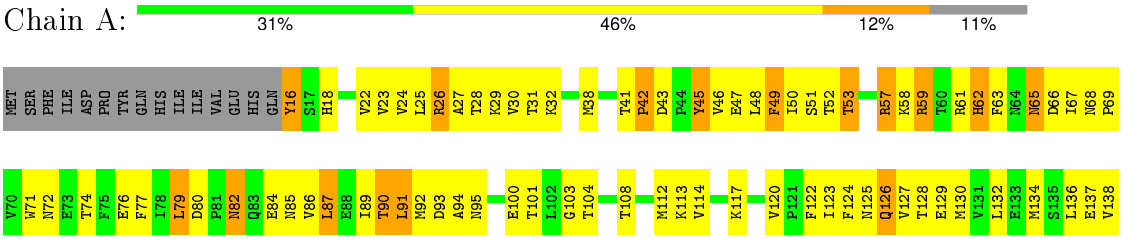
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

4 Residue-property plots (i)

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: CYTOSOLIC PHOSPHOLIPASE A2

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING, RESTRAINED MOLECULAR DYNAMICS, ETC.*.

Of the 75 calculated structures, 1 were deposited, based on the following criterion: *VIOLATION: NOES<0.3 A, DIHEDRAL ANGLES<3 DEGREES.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 4188
Number of chemical shift lists	1
Total number of shifts	1685
Number of shifts mapped to atoms	1685
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0	4
All	All	0	4

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	57	ARG	Sidechain
1	A	26	ARG	Sidechain
1	A	61	ARG	Sidechain
1	A	59	ARG	Sidechain

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	992	973	972	71
All	All	994	973	972	71

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

5 of 71 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:87:LEU:HD23	1:A:89:ILE:HD11	0.92	1.42
1:A:87:LEU:CD2	1:A:89:ILE:HD11	0.87	2.00
1:A:84:GLU:O	1:A:86:VAL:HG23	0.75	1.80
1:A:90:THR:HG23	1:A:104:THR:HB	0.72	1.59
1:A:123:ILE:HG23	1:A:128:THR:O	0.71	1.84

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	121/138 (88%)	83 (69%)	29 (24%)	9 (7%)	3 16
All	All	121/138 (88%)	83 (69%)	29 (24%)	9 (7%)	3 16

5 of 9 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	125	ASN
1	A	126	GLN
1	A	42	PRO
1	A	62	HIS
1	A	85	ASN

6.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	115/130 (88%)	92 (80%)	23 (20%)	5 36
All	All	115/130 (88%)	92 (80%)	23 (20%)	5 36

5 of 23 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency

of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	134	MET
1	A	53	THR
1	A	26	ARG
1	A	25	LEU
1	A	82	ASN

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4188

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1685
Number of shifts mapped to atoms	1685
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	137	-0.26 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	133	-0.08 ± 0.18	None needed (< 0.5 ppm)
$^{13}C'$	119	0.12 ± 0.17	None needed (< 0.5 ppm)
^{15}N	127	-0.38 ± 0.50	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 1333 atoms were assigned a chemical shift out of a possible 1521. 3 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	587/603 (97%)	239/240 (100%)	232/246 (94%)	116/117 (99%)
Sidechain	683/787 (87%)	420/456 (92%)	253/302 (84%)	10/29 (34%)

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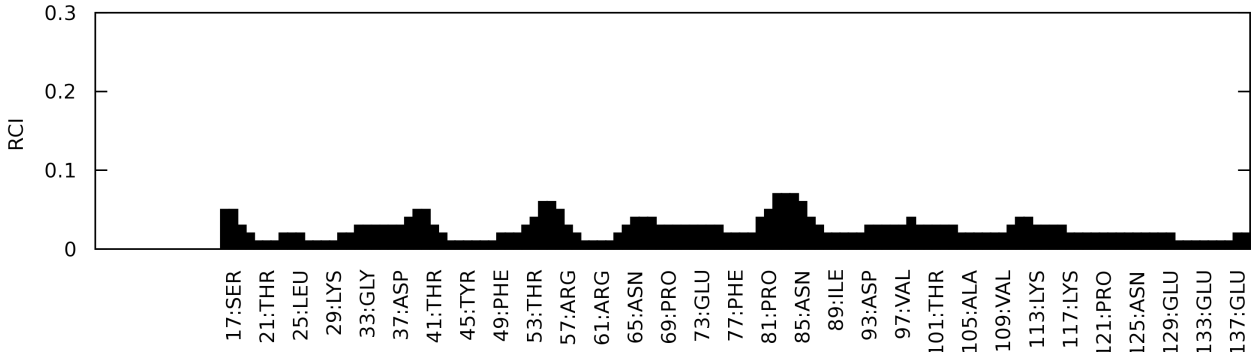
	Total	^{1}H	^{13}C	^{15}N
Aromatic	63/131 (48%)	41/71 (58%)	21/57 (37%)	1/3 (33%)
Overall	1333/1521 (88%)	700/767 (91%)	506/605 (84%)	127/149 (85%)

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	61	ARG	N	176.86	139.40 – 102.20	15.1
1	A	92	MET	HB3	-0.10	3.70 – 0.30	-6.2
1	A	69	PRO	HB3	-0.03	3.81 – 0.21	-5.7
1	A	43	ASP	HA	6.16	6.15 – 3.05	5.0

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: